

Adiabatic thermostatics of the two parameter entropy and the role of Lambert's W -function in its applications

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Abstract

A unified framework to describe the adiabatic class of ensembles in the generalized statistical mechanics based on Schwämmle-Tsallis two parameter (q, q') entropy is proposed. The generalized form of the equipartition theorem, virial theorem and the adiabatic theorem are derived. Each member of the class of ensembles is illustrated using the classical nonrelativistic ideal gas and we observe that the heat functions could be written in terms of the Lambert's W -function in the large N limit. We also noticed that negative specific heat exists for certain range of values of the deformation parameters. In the microcanonical ensemble we study the effect of gravitational field on classical nonrelativistic ideal gas and a system of hard rods in one dimension and compute their respective internal energy and specific heat.

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I Introduction

A system in thermodynamic equilibrium with its surroundings can be described using three macroscopic variables corresponding to the thermal, mechanical and the chemical equilibrium. For each fixed value of these macroscopic variables (macrostate) we have many possible microscopic configurations (microstates). A collection of systems existing in the various possible microstates but characterized by the same macroscopic variables is called an ensemble. The thermal, mechanical, and the chemical parameters can be chosen between either an extensive variable or an intensive variable and so, we have, in total eight different ensembles. The eight ensembles are further divided into two classes namely the isothermal class for which the thermal equilibrium variable is the temperature and the adiabatic class for which the thermal equilibrium variable is the heat function. The isothermal class comprises of the canonical (N, V, T) , isothermal-isobaric (N, P, T) , grandcanonical (μ, V, T) and the generalized ensemble (μ, P, T) . All the individual members of the adiabatic class of ensembles have same value for the heat function. The heat function is defined through the relation

$$\mathfrak{H} = E + \sum_{\{\ell\}} x_{\ell} X_{\ell}, \quad (1.1)$$

where E is the internal energy and the x is an intensive thermodynamic variable whose conjugate extensive variable is X . Defining \mathfrak{X}_1 and \mathfrak{X}_2 as the variables corresponding to the chemical and mechanical equilibrium the specific form for each ensemble, its heat function and the corresponding entropy are listed in the Table 1.

Table 1: List of Adiabatic ensembles

| ℓ | Ensemble | Heat function $\mathfrak{H} = E + \sum_{\{\ell\}} x_{\ell} X_{\ell}$ | Entropy $S(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H})$ |
|--------|---|---|--|
| 0 | Microcanonical (N, V, E) | E (Internal energy) | $S(N, V, E)$ |
| 1 | Isoenthalpic - isobaric (N, P, H) | $H = E + PV$ (Enthalpy) | $S(N, P, H)$ |
| 1 | Third adiabatic ensemble (μ, V, L) | $\mathsf{L} = E - \mu N$ (Hill energy) | $S(\mu, V, \mathsf{L})$ |
| 2 | Fourth adiabatic ensemble (μ, P, R) | $\mathsf{R} = E + PV - \mu N$ (Ray energy) | $S(\mu, P, \mathsf{R})$ |

Of the four adiabatic ensembles, the microcanonical and the isoenthalpic-isobaric ensembles described in [1-4] are well known, but the other two ensembles namely (μ, V, L) and (μ, P, R) introduced through References [5,6] are relatively less known. But they are important in studying adiabatically confined systems with variable number of particles. For example in Ref. [7] a Monte Carlo simulation of a system of liquid palladium has been carried out in the (μ, P, R) ensemble. The simulation was much more convenient in this ensemble and the results agreed with those obtained in the grandcanonical ensemble.

Realizing the importance of classifying the ensembles a unified treatment of the adiabatic ensembles was carried out in [8]. Later on the physical realizations corresponding to the eight ensembles and their interrelations through Laplace-Legendre transforms was studied in [9].

Tsallis proposed a generalization of the existing Boltzmann Gibbs statistical mechanics [10] through the introduction of q -deformed logarithm and exponential functions. The entropic expression in the generalized statistical mechanics was based on the q -deformed logarithm. Many other deformed entropies like the κ -entropy [11], the basic deformed entropies [12] etc., were also proposed. The equilibrium formulation of statistical mechanics based on the deformed entropies were developed and applied to a wide variety of systems like long range interacting rotators [13], relativistic gases [14,15], and systems with long range microscopic memory [16]. Classification of the eight ensembles in to two different classes namely, the isothermal and the adiabatic class, and a unified description for each class in the framework of generalized statistical mechanics based on Tsallis q entropy has been carried out in [17].

Later it was shown in [18] that an information theoretic entropy known as the Sharma-Taneja-Mittal entropy [19,20] based on a two parameter logarithm was a natural generalization of the κ -entropy. But the functional form of the two parameter exponential does not exist and so the distribution could not be written explicitly. With a view to provide a generalization of the Tsallis q entropy, a two parameter logarithm and its inverse function the two parameter exponential were introduced in [21]. The doubly deformed (q, q') logarithm and its inverse the (q, q') -exponential for a real variable x are

$$\ln_{q,q'}(x) = \frac{1}{1-q'} \left[\exp \left(\frac{1-q'}{1-q} (x^{1-q} - 1) \right) - 1 \right], \quad (1.2)$$

$$\exp_{q,q'}(x) = \left[1 + \frac{1-q}{1-q'} \ln(1 + (1-q')x) \right]^{\frac{1}{1-q}}. \quad (1.3)$$

The two parameter algebra based on the doubly deformed logarithm and the exponential was found [22] to be nondistributive in nature. Based on the definition of the two parameter logarithm (1.2) the generalized entropy is

$$\begin{aligned} S_{q,q'} &= k_{TS} \sum_{i=1}^w p_i \ln_{q,q'} \left(\frac{1}{p_i} \right), \\ &= \frac{k_{TS}}{1-q'} \sum_{i=1}^w p_i \left(\exp \left(\frac{1-q'}{1-q} (p_i^{q-1} - 1) \right) - 1 \right). \end{aligned} \quad (1.4)$$

Under the assumption of equiprobability i.e., $p_i = 1/w$ the two parameter entropy (1.4) reads:

$$S_{q,q'} = \frac{k_{TS}}{1-q'} \left(\exp \left(\frac{1-q'}{1-q} (w^{1-q} - 1) \right) - 1 \right). \quad (1.5)$$

Both the doubly deformed logarithm (1.2) and the exponential (1.3) reduce to the respective one parameter logarithm or exponential defined in [10], when we let either q or q' tend to unity. Due to this property, the Tsallis generalized entropy can be recovered by allowing either of the deformation parameters to approach it limiting value.

A canonical formulation of generalized statistical mechanics based on the two parameter entropy (1.4) was carried out in Ref. [23] and the authors found that the distribution could be obtained in terms of the Lambert's W -function. This can be formally extended to describe other members of the isothermal class of ensembles. In our current work we investigate the adiabatic class of ensembles of the generalized statistical mechanics based on the two parameter entropy. We provide a unified description of the adiabatic class and provide a two parameter generalization of the equipartition theorem, virial theorem and the adiabatic theorem. All the four ensembles are illustrated using the classical nonrelativistic ideal gas and their corresponding heat functions and heat capacities are obtained analytically. For the ideal gas, the phase space volume in the microcanonical and the isoenthalpic-isobaric ensemble can be found easily. To compute the respective heat function we need to adopt the large N limit and the results are obtained in terms of the Lambert's W -function. A brief introduction to the W -function is provided in Section II of this article. Corresponding to the (μ, V, L) and the (μ, P, R) ensembles the phase space volume could not be evaluated exactly and we overcome this by using the large N limit. Since the large N limit has been already used in the computation of the phase space volume no further approximations are needed in the calculation of the heat function and the specific heat. The effect of gravity on a classical nonrelativistic ideal gas, and a system of one dimensional hard rod gas has been investigated [24,25] in the extensive Boltzmann-Gibbs statistical mechanics. The authors found that the entropy is a decreasing function of the gravitational field indicating that gravity had an ordering effect in a thermodynamic system. In the present work we study the effect of a gravitational field in the framework of two parameter (q, q') entropy. First a D -dimensional nonrelativistic classical ideal gas confined in a finite region of space, subjected to an external gravitational field is investigated. The entropy and the specific heat are obtained exactly as a function of the internal energy. In the infinite height limit, the internal energy could be found only when we assume that the number of particles is very large. Next we study a system of one dimensional hard rods in the presence of gravity. Analogous to the classical ideal gas, the entropy and the specific heat are obtained as a function of internal energy. But in the infinite height limit the internal energy could be obtained as a function of temperature subject to the condition that the number of particles is very large.

The plan of the article is as follows: Following the introduction in Section I we give a brief summary of the Lambert's W function in Section II. A unified description of the thermostatistical structure of all the four adiabatic ensembles is provided in Section III. In Section IV, we study all the four ensembles using classical nonrelativistic ideal gas, and each ensemble is treated separately in a subsection. The effect of an external gravitational field on thermodynamic system is studied in Section V. The first part of the section deals with the effect of gravity on a D -dimensional classical ideal gas. A system of one dimensional hard rod gas is examined in second part of the section. The investigations are carried out in the microcanonical ensemble. We present our conclusions in Section V.

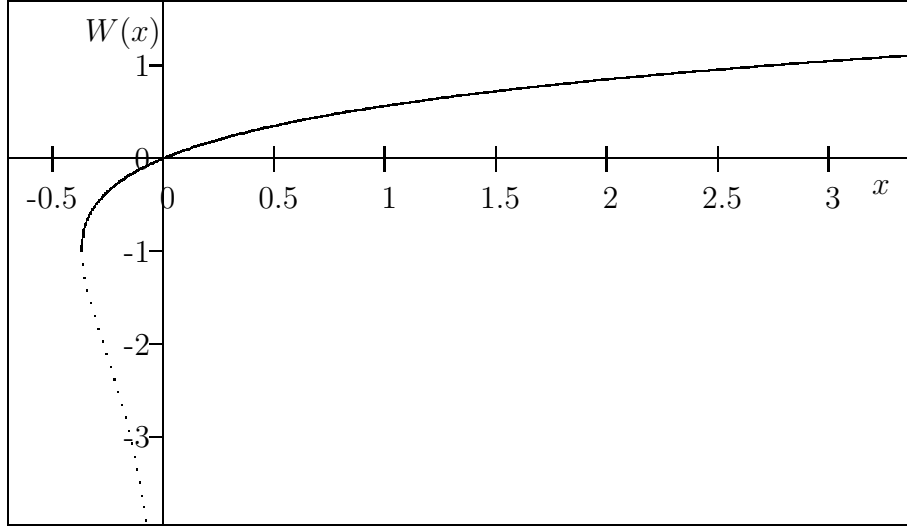


Figure 1: A plot of the Lambert's W function $W(x)$ as a function of x .

II Lambert's W -function: a primer

A brief summary of the Lambert's W -function and its mathematical properties is presented in the current section. Lambert's W -function represented by $W(z)$ is defined as the multivalued inverse of the function $w e^w = z$ and satisfies the relation

$$W(z) e^{W(z)} = z, \quad z \in \mathbb{C}. \quad (2.1)$$

The various branches corresponding to the W -function are indexed by $k = 0, \pm 1, \pm 2, \dots$, and for real $z < -1/e$, the function $W(z)$ is always complex and multivalued. For real z in the range $-1/e \leq z < 0$, the function $W(z)$ comprises of two real branches namely $W_0(z)$ and $W_{-1}(z)$ represented by the solid line and the dotted line respectively in Figure 1. The branch $W_0(z)$ satisfies the condition $W(z) \geq -1$, and is generally known as the principal branch of the W function. Correspondingly when $W(z) \leq -1$ we have the $W_{-1}(z)$ branch. The principal branch is analytic at $z = 0$ and has the series expansion

$$W_0(z) = \sum_{n=1}^{\infty} \frac{(-n)^{n-1}}{n!} z^n, \quad (2.2)$$

with a radius of convergence e^{-1} . Similarly the series corresponding to the branch W_{-1} is

$$W_{-1}(z) = \sum_{n=0}^{\infty} c_n f^n(z); \quad f(z) = \sqrt{2(ez + 1)}, \quad (2.3)$$

where the expansion coefficients can be computed from the recurrence relations

$$c_k = \frac{k-1}{k+1} \left(\frac{c_{k-2}}{2} + \frac{d_{k-2}}{4} \right) - \frac{d_k}{2} - \frac{c_{k-1}}{k+1}, \quad d_k = \sum_{j=2}^{k-1} c_j c_{k+1-j}, \quad (2.4)$$

$$c_0 = -1, \quad c_1 = 1, \quad d_0 = 2, \quad d_1 = -1. \quad (2.5)$$

The series converges for $-1/e \leq z < 0$, which covers the whole domain of the W_{-1} branch. From (2.1) the derivative of the W function can be found

$$W'(z) = \frac{W(z)}{z(1+W(z))}. \quad (2.6)$$

In the current article physical requirements restricts our choice of the W function to the principal branch. An excellent introduction to the Lambert's W -function and its applications to engineering problems is discussed in [26]. Recently in signal processing the role of the W_{-1} branch was analyzed [27]. The Lambert's function has been used in the study of both classical [28] and quantum statistical mechanics [29,30]. It also occurs [31] in the study of Fokker Planck equation in the small noise limit.

III Adiabatic ensemble: Generalized formulation

The individual members of an adiabatic ensemble have the same value of the heat function though they can be at different temperatures. For a system in thermodynamic equilibrium, there are four different adiabatic ensembles namely the microcanonical ensemble (N, V, U) , the isoenthalpic-isobaric ensemble (N, P, H) , the adiabatic ensemble with number fluctuations (μ, V, L) , and the adiabatic ensemble with both number and volume fluctuations (μ, P, R) . The microstate of a system of N particles can be represented by a single point in the $2DN$ dimensional phase space. Corresponding to a particular value of the heat function which is a macrostate, we have a huge number of microstates. We need to compute the total number of microstates since it is a measure of the entropy. The points denoting the microstate of the system lie so close to each other that the surface area of the constant heat function curve in the phase space is regarded as a measure of the total number of microstates. For a system described by a Hamiltonian \mathcal{H} the surface area corresponding to a constant heat function \mathfrak{H} curve can be calculated from

$$\Omega(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}) = \sum_{X_{\{\ell\}}} \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \delta\left(\mathcal{H} + \sum_{\{\ell\}} x_{\ell} X_{\ell} - \mathfrak{H}\right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (3.1)$$

Similarly the phase space volume enclosed by the constant heat function \mathfrak{H} curve is

$$\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}) = \sum_{X_{\{\ell\}}} \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \Theta\left(\mathcal{H} + \sum_{\{\ell\}} x_{\ell} X_{\ell} - \mathfrak{H}\right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (3.2)$$

Computation of the volume of the constant heat function curve assumes significance because of the difficulty in calculating the area of the curve. The volume enclosed by the phase space curve and its surface area are related via the expression

$$\Omega(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}) = \frac{\partial}{\partial \mathfrak{H}} \Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}). \quad (3.3)$$

Since the phase space volume is a measure of the number of the microstates of the system, the two parameter entropy can be directly obtained from the knowledge of $\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H})$ via the relation

$$S_{q,q'}(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}) = k \ln_{q,q'} \Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}). \quad (3.4)$$

For a given adiabatic ensemble the temperature is defined via the relation

$$T = \left(\frac{\partial S_{q,q'}}{\partial \mathfrak{H}} \right)^{-1} = \frac{(\Sigma(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}))^q}{k \Omega(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}) \exp \left(\frac{1-q'}{1-q} ((\Sigma(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}))^{1-q} - 1) \right)}. \quad (3.5)$$

Using the definition of the temperature (3.5), the phase space volume (3.2) and the surface area (3.1), we can calculate the expression corresponding to the heat function. From the expression for the heat function the specific heat can be calculated through the relation

$$C_{x_{\{\ell\}}} = \frac{\partial \mathfrak{H}_q}{\partial T} \Big|_{x_{\{\ell\}}}. \quad (3.6)$$

For any adiabatic ensemble the expectation value of an observable O is defined as

$$\langle O \rangle = \frac{1}{\Omega(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H})} \sum_{X_{\{\ell\}}} \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} O \delta \left(\mathcal{H} + \sum_{\{\ell\}} x_\ell X_\ell - \mathfrak{H} \right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (3.7)$$

The above expression is extremely useful in computing the average energy in the (N, P, H) , (μ, V, L) and the (μ, P, R) ensembles. By using the suitable Legendre transformations, the average energy can also be obtained from the heat functions corresponding to these ensembles. From the entropy the extensive thermodynamic quantities whose conjugate intensive variables are held fixed can be computed through the relation

$$X_\ell(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}) = -\frac{1}{\beta} \frac{\partial}{\partial x_\ell} S(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}). \quad (3.8)$$

The equipartition theorem is derived in a unified manner for all the four adiabatic ensembles in the framework of generalized statistical mechanics based on the Schwämmle-Tsallis (q, q') entropy. Representing the phase space variables r_i and p_i ($i = 1, 2, \dots, 3N$) by a common variable y_i , we find the following expectation value

$$\left\langle y_i \frac{\partial \mathcal{H}}{\partial y_j} \right\rangle = kT (\Sigma(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}))^{1-q} \exp \left(\frac{1-q'}{1-q} ((\Sigma(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}))^{1-q} - 1) \right) \delta_{ij}, \quad (3.9)$$

which is a generalization of the equipartition function. We notice that the (q, q') generalized equipartition theorem is dependent on the phase space volume in contrast to the extensive Boltzmann-Gibbs statistics. This observation is in line with the earlier result obtained for the Tsallis entropy in Ref. [17] and yields the Boltzmann-Gibbs limit when both the nonextensive parameters q and q' are set to unity. When we let the variable y_i to be the coordinate r_i and invoke the Dirac delta function, we get a specific form of the equipartition theorem:

$$\begin{aligned} \left\langle r_i \frac{\partial \mathcal{H}}{\partial r_i} \right\rangle &\equiv -\langle r_i \dot{p}_i \rangle = \langle r_i F_i \rangle = kT (\Sigma(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}))^{1-q} \\ &\exp \left(\frac{1-q'}{1-q} ((\Sigma(\mathfrak{X}_1, \mathfrak{X}_2, \mathfrak{H}))^{1-q} - 1) \right). \end{aligned} \quad (3.10)$$

Similarly when we set y_i to be equal to p_i the momentum variable we obtain

$$\left\langle p_i \frac{\partial \mathcal{H}}{\partial p_i} \right\rangle \equiv \langle p_i \dot{r}_i \rangle = kT (\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}))^{1-q} \exp \left(\frac{1-q'}{1-q} ((\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}))^{1-q} - 1) \right). \quad (3.11)$$

Through a canonical transformation, sometimes the Hamiltonian of a system can be written in the following form $\mathcal{H} = \sum_i A_i P_i^2 + B_i Q_i^2$. Aided by equations (3.10) and (3.11) we find the expectation value of such an Hamiltonian to be

$$\langle \mathcal{H} \rangle = DN kT (\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}))^{1-q} \exp \left(\frac{1-q'}{1-q} ((\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}))^{1-q} - 1) \right). \quad (3.12)$$

A two parametric generalization of the virial theorem could be obtained from the relation (3.10) and reads:

$$\left\langle \sum_i^{DN} r_i \dot{p}_i \right\rangle = -DN kT (\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}))^{1-q} \exp \left(\frac{1-q'}{1-q} ((\Sigma(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H}))^{1-q} - 1) \right). \quad (3.13)$$

Below we verify the adiabatic theorem for the generalized statistical mechanics based on the two parameter entropy. Let us consider the Hamiltonian to contain an external parameter a , in addition to the phase space co-ordinates. An expectation value of the derivative of the Hamiltonian with respect to the external parameter yields the thermodynamic conjugate variable f corresponding to the parameter a

$$\begin{aligned} \left\langle \frac{\partial \mathcal{H}}{\partial a} \right\rangle &= \frac{1}{\Omega(\mathfrak{x}_1, \mathfrak{x}_2, \mathfrak{H})} \sum_{X_\ell} \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \left(\frac{\partial \mathcal{H}}{\partial a} \right) \delta(\mathcal{H} + \sum_{X_\ell} x_\ell X_\ell - \mathfrak{H}) \prod_{i=1}^N d^D r_i d^D p_i, \\ &= \frac{\partial \mathfrak{H}}{\partial a} = f. \end{aligned} \quad (3.14)$$

The description of the adiabatic ensembles given above has been illustrated through certain examples. First we consider a classical ideal gas and provide an analytic solution to the specific heat in all the four ensembles by using a large N approximation. Later on we study a microcanonical D -dimensional classical ideal gas under the influence of gravity and compute its specific heat. Finally we investigate a hard rod gas under gravity in the framework of microcanonical ensemble.

IV Application - Classical ideal gas

The Hamiltonian of a nonrelativistic classical ideal gas in D dimensions is

$$\mathcal{H} = \sum_i \frac{p_i^2}{2m}, \quad p_i = |\mathbf{p}_i|, \quad (4.1)$$

where \mathbf{p}_i for $(i = 1, 2, \dots, N)$ represent the D -dimensional momenta of the gas molecules. In this section we find the phase space volume corresponding to this Hamiltonian for all the four ensembles. From the phase space volume we derive the relevant thermodynamic quantities like the entropy, the heat function and the heat capacity.

A. Microcanonical ensemble

The classical nonrelativistic ideal gas described by (4.1) is studied in the microcanonical ensemble. In order to compute the entropy of the system, we calculate the phase space volume enclosed by the constant energy curve. Substituting the expression of the Hamiltonian in (3.2)

$$\Sigma(N, V, E) = \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \Theta \left(\sum_i \frac{p_i^2}{2m} - E \right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (4.2)$$

The phase space integral is computed in the following manner: First we notice that the momentum integration is the volume of a DN -dimensional sphere of radius $\sqrt{2mE}$. Next we integrate over the position co-ordinates to obtain the phase space volume in the microcanonical ensemble

$$\Sigma(N, V, E) = \frac{V^N}{N!} \frac{\mathcal{M}^N}{\Gamma(\frac{DN}{2} + 1)} E^{\frac{DN}{2}}, \quad (4.3)$$

where we define $\mathcal{M} = (2\pi m/h^2)^{D/2}$ for the sake of convenience. The corresponding surface area enclosed by the phase space curve is

$$\Omega(N, V, E) = \frac{V^N}{N!} \frac{\mathcal{M}^N}{\Gamma(\frac{DN}{2})} E^{\frac{DN}{2}-1}. \quad (4.4)$$

The microcanonical entropy of a classical ideal gas obtained from the knowledge of the phase space volume (4.3) reads:

$$S_{q,q'} = \frac{k}{1-q'} \left[\exp \left(\frac{1-q'}{1-q} ((\Xi_{mc} E^{\frac{DN}{2}})^{1-q} - 1) \right) - 1 \right], \quad (4.5)$$

where the factor Ξ_{mc} is defined as

$$\Xi_{mc} = \frac{V^N}{N!} \frac{\mathcal{M}^N}{\Gamma(\frac{DN}{2} + 1)}. \quad (4.6)$$

In the limit $(q, q') \rightarrow 1$, we recover the extensive Boltzmann Gibbs entropy. From the definition of temperature (3.5), we arrive at the following expression

$$\frac{1}{T} = \frac{DN}{2} k \Xi_{mc}^{1-q} E^{(1-q)\frac{DN}{2}-1} \exp \left(\frac{1-q'}{1-q} ((\Xi_{mc} E^{\frac{DN}{2}})^{1-q} - 1) \right). \quad (4.7)$$

Inversion of the above relation (4.7), to obtain the internal energy is intractable and so, we look into the naturally occurring large N limit. In this limit we can safely neglect the factor of one in comparison with $(1-q)DN/2$ and this enables us to make the following approximation $E^{(1-q)\frac{DN}{2}-1} \approx E^{(1-q)\frac{DN}{2}}$. This is a valid approximation because, for very large values of N the deformation parameter $(1-q)$ should be $O(1/N)$ for the factor 1 to make a resonable contribution. Using the assumption outlined above we get

$$\exp \left(\frac{1-q'}{1-q} \right) \frac{2}{DN k T} = \Xi_{mc}^{1-q} E^{(1-q)\frac{DN}{2}} \exp \left(\frac{1-q'}{1-q} (\Xi_{mc} E^{\frac{DN}{2}})^{1-q} \right). \quad (4.8)$$

The inversion of the above function leads to an expression of the internal energy in terms of the Lambert's W function as

$$E = \left[\frac{1-q}{1-q'} \frac{1}{\Xi_{mc}^{1-q}} W_0 \left(\frac{1-q'}{1-q} \exp \left(\frac{1-q'}{1-q} \right) \frac{2\beta}{DN} \right) \right]^{\frac{2}{(1-q)DN}}. \quad (4.9)$$

The requirement that the entropy be concave decides the range of the deformation parameters. From the discussion in Ref. [21], we notice that the entropy is concave in the region $q + q' \geq 1$ excluding the region $0 \leq (q, q') \leq 1$, where the entropy does not have fixed curvature sign. The argument of the W function in (4.9) is positive in the region (a) for which $q > 1$ and $q' > 1$, and hence the energy in this region is characterized by the principal branch. Under the restriction $q + q' < 1$, there are two other major regions namely, (b) $q > 1$ and $-\infty < q' < 1$ and (c) $q' > 1$ and $-\infty < q < 1$ in which the argument of the W function is negative. Though we have a choice between the W_0 and the W_{-1} branch, the continuity requirement on energy restricts our choice to the W_0 branch. Thus we conclude that only the principal branch contributes in the definition of energy. In all the subsequent discussions in this article, we maintain the definition of the regions (a), (b) and (c) as described above. The specific heat at constant volume evaluated from the internal energy is

$$C_V \equiv \frac{\partial E}{\partial T} = -\frac{k\beta}{(1-q)DN/2} \frac{W_0(\mathbf{b}\beta)}{1+W_0(\mathbf{b}\beta)} [\mathbf{a} W_0(\mathbf{b}\beta)]^{\frac{1-(1-q)DN/2}{(1-q)DN/2}}, \quad (4.10)$$

where the factors \mathbf{a} and \mathbf{b} are as defined below:

$$\mathbf{a} = \frac{1-q}{1-q'} \frac{1}{\Xi_{mc}^{1-q}}, \quad \mathbf{b} = \frac{1-q'}{1-q} \exp \left(\frac{1-q'}{1-q} \right) \frac{2}{DN}. \quad (4.11)$$

Invoking the large N limit in the final expression of the specific heat we arrive at

$$C_V = -\frac{k\beta}{(1-q)DN/2} \frac{1}{\mathbf{a}(1+W_0(\mathbf{b}\beta))}. \quad (4.12)$$

From the expression of the specific heat (4.12), we notice that it can be either +ve or -ve depending on the values of the deformation parameters q and q' . In the region (a) and region (c) the specific heat is positive, whereas in the region (b) it is negative. We do not recover the Boltzmann Gibbs statistics from our above calculations, because in the computation of energy (4.9), we have made use of the large N limit which does not commute with extensive $(q, q') \rightarrow 1$ limit.

B. Isoenthalpic-isobaric ensemble

A system which exchanges internal energy and volume with its surroundings in such a way that its enthalpy remains constant is described by the isoenthalpic-isobaric ensemble. In order to calculate the thermodynamic quantities we first find the phase space volume enclosed by the constant enthalpy curve. The integral expression corresponding to the phase space volume is

$$\Sigma(N, P, H) = \sum_V \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \Theta \left(\sum_i \frac{p_i^2}{2m} + PV - H \right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (4.13)$$

Using the fact that the momentum integration is nothing but geometrically equivalent to a DN dimensional sphere of radius $\sqrt{2m(H - PV)}$, and integrating over the position co-ordinates we arrive at

$$\Sigma(N, P, H) = \frac{\mathcal{M}^N}{N!} \frac{1}{\Gamma\left(\frac{DN}{2} + 1\right)} \sum_V V^N (H - PV)^{\frac{DN}{2}}. \quad (4.14)$$

In the next step we consider a summation over the volume eigenstates. Since the volume states are very closely spaced the summation is replaced by an integration. But an integral over the volume leads to overcounting of the eigenstates. To overcome this we employ the shell particle method of counting volume states developed in [32,33]. In this method we take into account only the minimum volume needed to confine a particular configuration. The minimum volume needed to confine a particular configuration is found by imposing a condition wherein we require atleast one particle to lie on the boundary of the system. All the equivalent ways of choosing a minimum volume is treated as the same volume eigenstate and is considered only once. Using this shell particle technique to reject the redundant volume states we arrive at

$$\Sigma(N, P, H) = \mathcal{M}^N \left(\frac{1}{P}\right)^N \frac{H^{\mathfrak{D}}}{\Gamma(\mathfrak{D} + 1)}, \quad \mathfrak{D} = \frac{DN}{2} + N. \quad (4.15)$$

A similar evaluation of the surface area enclosed by the curve of constant enthalpy yields

$$\Omega(N, P, H) = \mathcal{M}^N \left(\frac{1}{P}\right)^N \frac{H^{\mathfrak{D}-1}}{\Gamma(\mathfrak{D})}. \quad (4.16)$$

From the knowledge of the phase space volume (4.15), the entropy of a classical ideal gas in the isenthalpic-isobaric ensemble is found:

$$S_{q,q'} = \frac{k}{1 - q'} \left[\exp \left(\frac{1 - q'}{1 - q} ((\Xi_{ie} H^{\mathfrak{D}})^{1-q} - 1) \right) - 1 \right]. \quad (4.17)$$

The Boltzmann Gibbs entropy is recovered in the limit $(q, q') \rightarrow 1$. The factor Ξ_{ie} used in the above equation is

$$\Xi_{ie} = \mathcal{M}^N \left(\frac{1}{P}\right)^N \frac{1}{\Gamma(\mathfrak{D} + 1)}. \quad (4.18)$$

The partial derivative of the entropy (4.17) with respect to the enthalpy gives the temperature of the isenthalpic-isobaric ensemble

$$\frac{1}{T} = \mathfrak{D} k \Xi_{ie}^{1-q} H^{(1-q)\mathfrak{D}-1} \exp \left(\frac{1 - q'}{1 - q} ((\Xi_{ie} H^{\mathfrak{D}})^{1-q} - 1) \right). \quad (4.19)$$

In order to invert the above equation we assume the large N limit and this consequently leads to the approximation that $H^{(1-q)\mathfrak{D}-1} \approx H^{(1-q)\mathfrak{D}}$. Rewriting the equation (4.19) based on the assumption yields the expression

$$\exp \left(\frac{1 - q'}{1 - q} \right) \frac{1}{\mathfrak{D} k T} = \Xi_{ie}^{1-q} H^{(1-q)\mathfrak{D}} \exp \left(\frac{1 - q'}{1 - q} (\Xi_{ie} H^{\mathfrak{D}})^{1-q} \right). \quad (4.20)$$

The solution of the above equation yields the enthalpy in terms of the Lambert's W -function

$$H = \left[\frac{1-q}{1-q'} \frac{1}{\Xi_{ie}^{1-q}} W_0 \left(\frac{1-q'}{1-q} \exp \left(\frac{1-q'}{1-q} \right) \frac{\beta}{\mathfrak{D}} \right) \right]^{\frac{1}{(1-q)\mathfrak{D}}}. \quad (4.21)$$

The requirement that the entropy should be concave, along with the fact that the enthalpy is a continuous function restricts our choice of the W function to the principal branch. The specific heat at constant pressure computed from the enthalpy (4.21) is

$$C_P \equiv \frac{\partial H}{\partial T} = - \frac{k\beta}{(1-q)\mathfrak{D}} \frac{W_0(\mathfrak{b}\beta)}{1+W_0(\mathfrak{b}\beta)} [\mathfrak{a} W_0(\mathfrak{b}\beta)]^{\frac{1-(1-q)\mathfrak{D}}{(1-q)\mathfrak{D}}}, \quad (4.22)$$

where, the factors \mathfrak{a} and \mathfrak{b} are as defined below:

$$\mathfrak{a} = \frac{1-q}{1-q'} \frac{1}{\Xi_{ie}^{1-q}}, \quad \mathfrak{b} = \frac{1-q'}{1-q} \exp \left(\frac{1-q'}{1-q} \right) \frac{1}{\mathfrak{D}}. \quad (4.23)$$

In the large N limit the expression for the heat capacity reads:

$$C_P = - \frac{k\beta}{(1-q)\mathfrak{D}} \frac{1}{\mathfrak{a}(1+W_0(\mathfrak{b}\beta))}. \quad (4.24)$$

The specific heat is positive in the regions (a) and (c) and negative in the region (b). Since we adopted the large N limit in evaluating the enthalpy (4.21) we do not recover the corresponding Boltzmann Gibbs result, because the extensive limit and the large N limit do not commute with each other.

C. (μ, V, L) ensemble

The Hill energy L is the heat function corresponding to the (μ, V, L) ensemble. The phase space volume enclosed by the curve of constant Hill energy L is

$$\Sigma(\mu, V, \mathsf{L}) = \sum \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \Theta \left(\sum_i \frac{p_i^2}{2m} - \mu N - \mathsf{L} \right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (4.25)$$

Integrating over the phase space variables p_i and r_i , we arrive at

$$\Sigma(\mu, V, \mathsf{L}) = \sum_{N=0}^{\infty} \frac{V^N}{N!} \frac{\mathcal{M}^N}{\Gamma(\frac{DN}{2} + 1)} (\mathsf{L} + \mu N)^{\frac{DN}{2}}. \quad (4.26)$$

An exact evaluation of the summation given in (4.26) could not be achieved. In order to calculate an approximate value in the large N limit we carry out the following procedure. First we approximate the factor $(\mathsf{L} + \mu N)^{\frac{DN}{2}}$ as follows

$$\begin{aligned} (\mathsf{L} + \mu N)^{\frac{DN}{2}} &= (\mu N)^{\frac{DN}{2}} \left(1 + \frac{\mathsf{L}}{\mu N} \right)^{\frac{DN}{2}}, \\ &= (\mu N)^{\frac{DN}{2}} \exp \left(\frac{DN}{2} \ln \left(1 + \frac{\mathsf{L}}{\mu N} \right) \right). \end{aligned} \quad (4.27)$$

For very small values of x we can make use of the approximation $\ln(1+x) \approx x$ and this leads to

$$(\mathbb{L} + \mu N)^{\frac{DN}{2}} = (\mu N)^{\frac{DN}{2}} \exp\left(\frac{D}{2} \frac{\mathbb{L}}{\mu}\right). \quad (4.28)$$

In the next step we use the Stirling's approximation for the gamma function as given below:

$$\Gamma\left(\frac{DN}{2} + 1\right) \approx \left(\frac{DN}{2}\right)^{\frac{DN}{2}} \exp\left(-\frac{DN}{2}\right). \quad (4.29)$$

Substituting the relations (4.28), and (4.29) in (4.26) we arrive at

$$\Sigma(\mu, V, \mathbb{L}) = \exp\left(\frac{D}{2} \frac{\mathbb{L}}{\mu}\right) \sum_{N=0}^{\infty} \frac{V^N}{N!} \frac{\mathcal{M}^N}{\left(\frac{DN}{2}\right)^{\frac{DN}{2}} \exp\left(-\frac{DN}{2}\right)} (\mu N)^{\frac{DN}{2}}. \quad (4.30)$$

Now the summation over N can be carried out in (4.30), enabling us to write the approximate expression for the phase space volume

$$\Sigma(\mu, V, \mathbb{L}) = \exp\left(\frac{D}{2} \frac{\mathbb{L}}{\mu}\right) \exp\left(\frac{V \mu^{D/2} e^{D/2} \mathcal{M}}{(D/2)^{D/2}}\right). \quad (4.31)$$

The approximate computation used by us to calculate the phase space volume (4.31) can be considered as a first order approximation of the summation in (4.26). Similarly the surface area enclosed by the curve of constant \mathbb{L} is also found

$$\Omega(\mu, V, \mathbb{L}) = \frac{D}{2\mu} \exp\left(\frac{D}{2} \frac{\mathbb{L}}{\mu}\right) \exp\left(\frac{V \mu^{D/2} e^{D/2} \mathcal{M}}{(D/2)^{D/2}}\right). \quad (4.32)$$

The entropy of the classical ideal gas in this adiabatic ensemble found from (4.31) is

$$S_{q,q'} = \frac{k}{1-q'} \left[\exp\left(\frac{1-q'}{1-q} \left(\left(\Xi_{he} \exp\left(\frac{D}{2} \frac{\mathbb{L}}{\mu}\right) \right)^{1-q} - 1 \right) \right) - 1 \right], \quad (4.33)$$

where, for the sake of convenience we define:

$$\Xi_{he} = \exp\left(\frac{V \mu^{D/2} e^{D/2} \mathcal{M}}{(D/2)^{D/2}}\right). \quad (4.34)$$

The temperature of this ensemble calculated from the defining relation (3.5) is

$$\frac{1}{T} = \frac{D}{2\mu} k \Xi_{he}^{1-q} \left(\exp\left(\frac{D}{2} \frac{\mathbb{L}}{\mu}\right) \right)^{1-q} \exp\left(\frac{1-q'}{1-q} \left(\left(\Xi_{he} \exp\left(\frac{D}{2} \frac{\mathbb{L}}{\mu}\right) \right)^{1-q} - 1 \right) \right). \quad (4.35)$$

Rewriting (4.35) we immediately recognize it as the equation whose solution is given by the Lambert's W -function. Thus the Hill energy in terms of the W -function reads:

$$\mathbb{L} = \frac{2\mu}{(1-q)D} \ln \left[\frac{1-q}{1-q'} \frac{1}{\Xi_{he}^{1-q}} W_0 \left(\frac{1-q'}{1-q} \exp\left(\frac{1-q'}{1-q}\right) \frac{2\beta\mu}{D} \right) \right]. \quad (4.36)$$

The principal branch of the W function is chosen based on the concavity requirement on the entropy and the continuity of the Hill energy. The Hill energy \mathcal{L} is uniformly positive in the region (c) for which $q' > 1$ and $-\infty < q < 1$, whereas in the other two regions (b) and (c) it is positive only when the argument of the logarithm is less than 1. From (4.36) the specific heat at constant volume is found

$$C_V \equiv \frac{\partial \mathcal{L}}{\partial T} = -\frac{\mu}{(1-q)D/2} \frac{k\beta}{1+W_0(\mathfrak{b}\beta)}, \quad \mathfrak{b} = \frac{1-q'}{1-q} \exp\left(\frac{1-q'}{1-q}\right) \frac{\mu}{D/2}. \quad (4.37)$$

Subject to the condition $q + q' > 1$ and excluding the region $0 \leq (q, q') \leq 1$, the specific heat is +ve in the region $q > 1$ and -ve in the region $q < 1$. Due to the noncommutative nature of the extensive limit and the large N limit, we are unable to Boltzmann Gibbs result corresponding to the Hill energy (4.36) and the heat capacity (4.37).

D. (μ, P, \mathcal{R}) ensemble

The adiabatic ensemble with both the number and volume fluctuations is illustrated using the classical ideal gas in this section. The phase space volume of the classical ideal gas in this ensemble is

$$\Sigma(\mu, P, \mathcal{R}) = \sum_N \sum_V \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \Theta\left(\sum_i \frac{p_i^2}{2m} + PV - \mu N - \mathcal{R}\right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (4.38)$$

Integrating over the phase space co-ordinates namely p_i and r_i we arrive at

$$\Sigma(\mu, P, \mathcal{R}) = \sum_{N=0}^{\infty} \sum_V \frac{V^N}{N!} \frac{\mathcal{M}^N}{\Gamma\left(\frac{DN}{2} + 1\right)} (\mathcal{R} + \mu N - PV)^{\frac{DN}{2}}. \quad (4.39)$$

The sum over volume eigenstates is calculated by approximating it to an integral. Since a direct integration will lead to overcounting of the volume states, we use the shell particle method of counting which was developed in [32,33]. Using this technique eliminates the redundant volume states and the expression for the phase space volume after due evaluation is

$$\Sigma(\mu, P, \mathcal{R}) = \sum_{N=0}^{\infty} \mathcal{M}^N \left(\frac{1}{P}\right)^N \frac{(\mathcal{R} + \mu N)^{\mathfrak{D}}}{\Gamma(\mathfrak{D} + 1)}. \quad (4.40)$$

Finally we evaluate the summation over the number of particles in (4.40) using a large N approximation. The large N limit of the $(\mathcal{R} + \mu N)^{\mathfrak{D}}$ factor is calculated as follows

$$(\mathcal{R} + \mu N)^{\mathfrak{D}} = (\mu N)^{\mathfrak{D}} \left(1 + \frac{\mathcal{R}}{\mu N}\right)^{\mathfrak{D}} = (\mu N)^{\mathfrak{D}} \exp\left(\mathfrak{D} \ln\left(1 + \frac{\mathcal{R}}{\mu N}\right)\right). \quad (4.41)$$

Using the approximation $\ln(1+x) \approx x$ for small values of x we get

$$(\mathcal{R} + \mu N)^{\mathfrak{D}} = (\mu N)^{\mathfrak{D}} \exp\left(\frac{\mathfrak{D} \mathcal{R}}{\mu}\right). \quad (4.42)$$

Based on the Stirling's approximation the Gamma function in (4.40) is written as

$$\Gamma(\mathfrak{D} + 1) \approx \mathfrak{D}^{\mathfrak{D}} \exp(-\mathfrak{D}). \quad (4.43)$$

Substituting (4.42) and (4.43), we can rewrite (4.40) as follows

$$\Sigma(\mu, P, R) = \exp\left(\frac{\mathcal{D}R}{\mu}\right) \sum_{N=0}^{\infty} \left(\frac{\mathcal{M}}{P}\right)^N \left(\frac{\mu}{\mathcal{D}}\right)^{\mathfrak{D}} \exp(\mathfrak{D}), \quad (4.44)$$

where $\mathcal{D} = \mathfrak{D}/N$. Carrying out the summation in (4.44) we get the final expression of the phase space volume in the large N limit

$$\Sigma(\mu, P, R) = \exp\left(\frac{\mathcal{D}R}{\mu}\right) \left[1 - \frac{\mathcal{M}}{P} \left(\frac{\mu}{\mathcal{D}}\right)^{\mathcal{D}} \exp(\mathcal{D})\right]^{-1}. \quad (4.45)$$

The computed phase space volume (4.45) can be considered as a first order approximation of (4.40). The surface area of the phase space curve is

$$\Omega(\mu, P, R) = \frac{\mathcal{D}}{\mu} \exp\left(\frac{\mathcal{D}R}{\mu}\right) \left[1 - \frac{\mathcal{M}}{P} \left(\frac{\mu}{\mathcal{D}}\right)^{\mathcal{D}} \exp(\mathcal{D})\right]^{-1}. \quad (4.46)$$

The two parameter entropy of the classical ideal gas in the (μ, P, R) ensemble can be immediately obtained from the phase space volume (4.45) and reads:

$$S_{q,q'} = \frac{k}{1-q'} \left[\exp\left(\frac{1-q'}{1-q} \left(\left(\Xi_{re} \exp\left(\frac{\mathcal{D}R}{\mu}\right) \right)^{1-q} - 1 \right) \right) - 1 \right], \quad (4.47)$$

where the temperature independent factor Ξ_{re} of (4.47) is

$$\Xi_{re} = \left[1 - \frac{\mathcal{M}}{P} \left(\frac{\mu}{\mathcal{D}}\right)^{\mathcal{D}} \exp(\mathcal{D})\right]^{-1}. \quad (4.48)$$

The temperature of the (μ, P, R) ensemble is

$$\frac{1}{T} \equiv \frac{\partial S_{q,q'}}{\partial R} = \frac{\mathcal{D}}{\mu} \Xi_{re}^{1-q} \left(\exp\left(\frac{\mathcal{D}R}{\mu}\right) \right)^{1-q} \exp\left(\frac{1-q'}{1-q} \left(\left(\Xi_{re} \exp\left(\frac{\mathcal{D}R}{\mu}\right) \right)^{1-q} - 1 \right) \right). \quad (4.49)$$

Inverting the expression for the temperature in (4.49) helps us in computing the Ray energy, the heat function corresponding to the (μ, P, R) ensemble. The expression for the Ray energy of the classical ideal gas reads:

$$R = \frac{\mu}{(1-q)\mathcal{D}} \ln \left[\frac{1-q}{1-q'} \frac{1}{\Xi_{re}^{1-q}} W_0 \left(\frac{1-q'}{1-q} \exp\left(\frac{1-q'}{1-q} \frac{\beta\mu}{\mathcal{D}}\right) \right) \right]. \quad (4.50)$$

The continuity requirement of the Ray energy R , and the concavity conditions on the entropy restricts our choice of the W -function to the principal branch. In the region (c) for which $q' > 1$ and $-\infty < q < 1$ the Ray energy is uniformly positive whereas in the

other two regions *viz* (a) and (b) it is positive only when the argument of the logarithm is less than 1. From (4.50) the specific heat at constant pressure is found:

$$C_P \equiv \frac{\partial R}{\partial T} = -\frac{\mu}{(1-q)\mathcal{D}} \frac{k\beta}{1+W_0(\mathbf{b}\beta)}, \quad \mathbf{b} = \frac{1-q'}{1-q} \exp\left(\frac{1-q'}{1-q}\right) \frac{\mu}{\mathcal{D}}. \quad (4.51)$$

Analogous to the (μ, V, L) the specific heat is positive in the region $q < 1$ and negative in the region $q > 1$ under the condition that $q + q' > 1$ and excluding the region $0 \leq (q, q') \leq 1$. Further the Boltzmann Gibbs results could not be recovered from (4.50) and (4.51) since we have used the large N limit in the computation of the density of states and it does not commute with the extensive $(q, q') \rightarrow 1$ limit.

V Gas molecules under gravity

In order to investigate the effect of an external field on a thermodynamic system we study a system of gas molecules in the presence of a gravitational field in the current section. A system of D -dimensional classical ideal gas under the effect of gravity is explored in the first part of the section. To understand an interacting system in an external field, we, in the later part of the section, examine a system of hard rods confined in a linear box of length L in the presence of an external gravitational field.

A. D -dimensional ideal gas under gravity

A system of N noninteracting classical point-like particles of mass m is considered in D -dimensions in the presence of a uniform gravitational field g . The acceleration due to gravity acts along one of the dimensions labeled as the z co-ordinate and the force is oriented in a direction opposite to that of the co-ordinate axis. To conform to reality we consider that the gas molecules are located within a fixed region in space and so the position co-ordinates take values over a finite interval. Of the D position co-ordinates denoted by r_i ($i = 1, 2, \dots, D$), the z co-ordinate ranges over the interval $(0, H)$ and the remaining $D - 1$ co-ordinates range over the values $(0, L)$. The Hamiltonian of the D -dimensional ideal gas under gravity is

$$\mathcal{H} = \sum_{i=1}^{DN} \frac{p_i^2}{2m} + \sum_{j=1}^N mgz_j + U. \quad (5.1)$$

The fact that the gas molecules are to exist within a finite region in space is indicated in the Hamiltonian through a potential which mimics the presence of a wall

$$U = \begin{cases} 0 & \text{within the allowed region,} \\ \infty & \text{outside the allowed region.} \end{cases} \quad (5.2)$$

Substituting the expression for the Hamiltonian (5.1) in the integral for the phase space volume enclosed by a constant energy curve, we arrive at

$$\Sigma(N, V, E) = \frac{1}{N! h^{DN}} \int_{r_i} \int_{p_i} \Theta \left(\sum_{i=1}^{DN} \frac{p_i^2}{2m} + \sum_{j=1}^N mgz_j + U - E \right) \prod_{i=1}^N d^D r_i d^D p_i. \quad (5.3)$$

Integrating over the phase space co-ordinates, the volume enclosed by the constant energy curve is

$$\Sigma(N, V, E) = \frac{V^N}{N! h^{DN}} \frac{\mathcal{M}^N}{\Gamma(\mathfrak{D} + 1) (mgH)^N} \mathfrak{S}_D(E, mgH), \quad (5.4)$$

where $\mathfrak{S}(a, b)$ is a finite sum defined as below:

$$\mathfrak{S}_D(a, b) = \sum_{k=0}^N (-1)^k \binom{N}{k} (a - kb)^{\mathfrak{D}} \Theta(a - kb). \quad (5.5)$$

The surface area of the constant energy curve in the phase space is

$$\Omega(N, V, E) = \frac{V^N}{N! h^{DN}} \frac{\mathcal{M}^N}{\Gamma(\mathfrak{D}) (mgH)^N} \mathfrak{S}'_D(E, mgH), \quad (5.6)$$

where the prime over the summation (5.5) denotes a partial derivative with respect to the energy. Substituting the phase space volume (5.4) in equation (3.4) we obtain the entropy of a D -dimensional ideal gas in the presence of gravity

$$S_{q,q'} = \frac{k}{1 - q'} \left[\exp \left(\frac{1 - q'}{1 - q} ((\Xi_g \mathfrak{S}_D(E, mgH))^{1-q} - 1) \right) - 1 \right], \quad (5.7)$$

where, the factor Ξ_g is defined as

$$\Xi_g = \frac{A^N}{N! h^{DN}} \frac{\mathcal{M}^N}{\Gamma(\mathfrak{D} + 1) (mgH)^N}, \quad A = \prod_{\alpha=1}^{D-1} L_{\alpha}. \quad (5.8)$$

Using the entropic expression (5.7) and from the definition of temperature (3.5) we get

$$\frac{1}{T} = k \Xi_g^{1-q} \frac{\mathfrak{S}'_D(E, mgH)}{(\mathfrak{S}_D(E, mgH))^q} \exp \left(\frac{1 - q'}{1 - q} ((\Xi_g \mathfrak{S}_D(E, mgH))^{1-q} - 1) \right). \quad (5.9)$$

Looking at the structure of the relation (5.9) given above we realize that an inversion to obtain the internal energy as a function of temperature is not feasible. But the specific heat of the system can also be computed from the knowledge of the phase space volume (5.4) and the surface area (5.6) and the temperature (5.9) via the relation:

$$C_V \equiv \left(\frac{\partial T}{\partial E} \right)^{-1} = \left[T \left(\frac{q}{\Sigma} \Omega - \frac{1}{\Omega} \frac{\partial \Omega}{\partial E} - (1 - q') \frac{\Omega}{\Sigma^q} \right) \right]^{-1}. \quad (5.10)$$

Substituting the phase space volume (5.4), area of the curve (5.6) and the expression for the temperature (5.9) in (5.10) the specific heat as a function of temperature reads:

$$C_V = \mathfrak{D} k \exp \left(\frac{1 - q'}{1 - q} ((\Xi_g \mathfrak{S}_D(E, mgH))^{1-q} - 1) \right) \left[\mathfrak{D} q (\Xi_g \mathfrak{S}_D(E, mgH))^{q-1} - \Xi_g^{q-1} \frac{(\mathfrak{S}_D(E, mgH))^q}{\mathfrak{S}'_D(E, mgH)} \frac{\partial}{\partial E} \ln \mathfrak{S}'_D(E, mgH) - (1 - q') \mathfrak{D} \right]^{-1}. \quad (5.11)$$

From (5.11) it can be noticed that the specific heat can have both +ve and -ve values depending on the term in square bracket. We investigate the relevant limiting cases: (i) First is the $g \rightarrow 0$ limit in which the gas molecules behave like an ideal gas. (ii) The second case is the $H \rightarrow \infty$ limit in which the (5.9) can be inverted in the large N limit to obtain the energy as a function of temperature. We present the relevant calculation of this limiting case in the discussion below:

In the infinite height limit the limiting value of the summation (5.5) and its derivative are

$$\lim_{H \rightarrow \infty} \mathfrak{S}_D(E, mgH) = E^{\mathfrak{D}}, \quad \lim_{H \rightarrow \infty} \mathfrak{S}'_D(E, mgH) = \mathfrak{D} E^{\mathfrak{D}-1}. \quad (5.12)$$

Substitution of the limiting value (5.12) in the expression for the temperature (5.9) leads to:

$$\frac{1}{kT} = \mathfrak{D} k \Xi_g^{1-q} E^{(1-q)\mathfrak{D}-1} \exp\left(\frac{1-q'}{1-q} ((\Xi_g E^{\mathfrak{D}})^{1-q} - 1)\right). \quad (5.13)$$

In the large N limit using the approximation $E^{(1-q)\mathfrak{D}-1} \approx E^{(1-q)\mathfrak{D}}$ in (5.13), we can invert it to obtain the internal energy as a function of temperature in terms of the Lambert's W-function

$$E = \left[\frac{1-q}{1-q'} \frac{1}{\Xi_g^{1-q}} W_0\left(\frac{1-q'}{1-q} \exp\left(\frac{1-q'}{1-q}\right) \frac{\beta}{\mathfrak{D}}\right) \right]^{\frac{1}{(1-q)\mathfrak{D}}}. \quad (5.14)$$

The preconditions that the entropy should be concave, and the energy should be a continuous function helps us to conclude that only the principal branch of the W function occurs in (5.14). The specific heat of the classical ideal gas under gravity computed from the internal energy is

$$C_V = -\frac{k\beta}{(1-q)\mathfrak{D}} \frac{W_0(\mathfrak{b}\beta)}{1+W_0(\mathfrak{b}\beta)} [\mathfrak{a}_g W_0(\mathfrak{b}\beta)]^{\frac{1-(1-q)\mathfrak{D}}{(1-q)\mathfrak{D}}}, \quad (5.15)$$

where the factor \mathfrak{b} was introduced in (4.23) and \mathfrak{a}_g is

$$\mathfrak{a}_g = \frac{1-q}{1-q'} \frac{1}{\Xi_g^{1-q}}. \quad (5.16)$$

The large N limit of the specific heat for the ideal gas under gravity reads:

$$C_V = -\frac{k\beta}{(1-q)\mathfrak{D}} \frac{1}{\mathfrak{a}_g(1+W_0(\mathfrak{b}\beta))}. \quad (5.17)$$

Investigating the expression for the specific heat, we find that it can be either +ve in the regions (a) and (c) or -ve in the region (b). Since we have already made use of the large N limit we do not recover the Boltzmann Gibbs results because the thermodynamic limit and the extensive limit do not commute with each other.

The one parameter limits corresponding to the temperature relation (5.9) can be obtained by allowing either q or q' to take the limiting value. We notice that the expression for the temperature is the same when we set either of the parameter to unity and reads:

$$\frac{1}{T} = k \Xi_g^{1-q} \frac{\mathfrak{S}_D(E, mgH)}{\mathfrak{S}'_D(E, mgH)}. \quad (5.18)$$

The definition of temperature (5.18) can be inverted to obtain the internal energy and the specific heat in the $H \rightarrow \infty$ limit, but there is no need to invoke the large N limit.

B. 1D hard rod gas under gravity

The generalized statistical mechanics based on the two parameter (q, q') entropy is applied to a system comprising of N one dimensional hard rods under gravity. Initially we consider a system of hard rods of mass m and length σ in a finite region of the space under the influence of a uniform gravitational field of strength g . The position of the centers and the momentum of the hard rods are denoted by the set of values $(z_1, \dots, z_N; p_1, \dots, p_N)$. Two rods with centers given by z_0 and z_{N+1} are considered so that their edges define the boundaries of the region, in such way that $z_{N+1} - z_0 = L + \sigma$. The relevant thermodynamic quantities like the entropy, the temperature and the heat capacity are then computed. Later we assume $L \rightarrow \infty$ limit of the system and obtain the internal energy in this limiting case. The Hamiltonian of a one dimensional hard rod gas under gravity reads:

$$\mathcal{H} = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i=1}^N mgz_i + \sum_{i < j} u(|z_j - z_i|) + \sum_{i=1}^N U(z_i; z_0, z_{N+1}). \quad (5.19)$$

The distance between the centers of any two particles in the system cannot be less than the length of the rod σ and the potential corresponding to it is

$$u(|z_j - z_i|) = \begin{cases} \infty, & |z_j - z_i| < \sigma, \\ 0, & |z_j - z_i| \geq \sigma. \end{cases} \quad (5.20)$$

Similarly the existence of the gas molecules within the finite region of the space is indicated in the Hamiltonian (5.19) via the potential

$$U = \begin{cases} 0, & z_0 + \sigma \leq z_i \leq z_{N+1} - \sigma, \\ \infty, & \text{otherwise.} \end{cases} \quad (5.21)$$

Using the Hamiltonian (5.19) in (3.2), the integral expression corresponding to the phase space volume is

$$\Sigma(N, L, E) = \frac{1}{N! h^N} \int_{z_i} \int_{p_i} \Theta \left(\sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{j=1}^N mgz_j + U + u(|z_j - z_i|) - E \right) \prod_{i=1}^N dz_i dp_i. \quad (5.22)$$

To evaluate the phase space volume we first integrate over the momentum variables. In the next step we use the substitution $r_k = z_k - (z_0 + k\sigma)$ for the position integrals which helps us in integrating over the position variables. The final expression for the phase space volume thus computed is

$$\Sigma(N, L, E) = \frac{\mathcal{M}_1^N}{N! \Gamma\left(\frac{3N}{2} + 1\right) (mg)^N} \mathfrak{S}_1(E - mg\alpha, mg\bar{L}). \quad (5.23)$$

where the \mathcal{M}_1 is the one dimensional equivalent of \mathcal{M} . For convenience we have also defined the following quantities

$$\alpha = Nz_0 + \frac{N(N+1)}{2} \sigma, \quad \bar{L} = L - N\sigma. \quad (5.24)$$

The surface area of the constant energy curve is

$$\Omega(N, L, E) = \frac{\mathcal{M}_1^N}{N! \Gamma\left(\frac{3N}{2}\right) (mg)^N} \mathfrak{S}'_1(E - mg\alpha, mg\bar{L}). \quad (5.25)$$

The knowledge of the phase space volume (5.23) enables us to obtain the entropy of the system defined through the relation (3.4). Combining this with the definition of temperature (3.5), we arrive at

$$\frac{1}{T} = k \Xi_{gh}^{1-q} \frac{\mathfrak{S}'_1(E - mg\alpha, mg\bar{L})}{(\mathfrak{S}_1(E - mg\alpha, mg\bar{L}))^q} \exp\left(\frac{1-q'}{1-q} ((\Xi_{gh} \mathfrak{S}_1(E - mg\alpha, mg\bar{L}))^{1-q} - 1)\right), \quad (5.26)$$

where the factor Ξ_{gh} is defined as

$$\Xi_{gh} = \frac{\mathcal{M}_1^N}{N! \Gamma\left(\frac{3N}{2} + 1\right) (mg)^N}. \quad (5.27)$$

The form of (5.26) makes us realize that an exact inversion to obtain the internal energy is not feasible. To overcome this we use (5.10) in conjunction with (5.23), (5.25) and (5.26) to compute the specific heat as a function of the internal energy and the free length (\bar{L}). The specific heat thus evaluated is

$$\begin{aligned} C_V = & \frac{3N}{2} k \exp\left(\frac{1-q'}{1-q} ((\Xi_{gh} \mathfrak{S}_1(E - mg\alpha, mg\bar{L}))^{1-q} - 1)\right) \\ & \left[\frac{3N}{2} q (\Xi_{gh} \mathfrak{S}_1(E - mg\alpha, mg\bar{L}))^{q-1} \right. \\ & \left. - \Xi_{gh}^{q-1} \frac{(\mathfrak{S}_1(E - mg\alpha, mg\bar{L}))^q}{\mathfrak{S}'_1(E - mg\alpha, mg\bar{L})} \frac{\partial}{\partial E} \ln \mathfrak{S}'_1(E - mg\alpha, mg\bar{L}) - (1-q') \frac{3N}{2} \right]^{-1}. \end{aligned} \quad (5.28)$$

Analyzing (5.28) we realize that both positive and negative values of specific heat are permissible depending on the argument within the square bracket. There are two pertinent limiting cases namely (i) the $g \rightarrow 0$ limit wherein it becomes a system of hard rods moving in a length L , and (ii) the $L \rightarrow \infty$ limit. In the second limit we present the expression for temperature below:

$$\frac{1}{T} = \frac{3N}{2} k \Xi_{gh}^{1-q} (E - mg\alpha)^{(1-q)\frac{3N}{2}-1} \exp\left(\frac{1-q'}{1-q} \left((\Xi_{gh} (E - mg\alpha)^{\frac{3N}{2}})^{1-q} - 1\right)\right), \quad (5.29)$$

which can be inverted in the large N limit by assuming $(3N/2) - 1 \approx (3N/2)$. This approximation yields the internal energy in terms of the Lambert's W -function

$$E = \left[\frac{1-q}{1-q'} \frac{1}{\Xi_{gh}^{1-q}} W_0\left(\frac{1-q'}{1-q} \exp\left(\frac{1-q'}{1-q}\right) \frac{2\beta}{3N}\right) \right]^{\frac{2}{(1-q)3N}} + mg\alpha. \quad (5.30)$$

The stipulations that the entropy should be concave and the energy should be a continuous function limits us to the principal branch of the W -function. The specific heat of the hard

rod gas in the large N limit can be obtained from (5.30) and has the same regimes of positive and negative specific heat values as the classical ideal gas.

The one parameter limits of the temperature (5.26) is investigated. It can be noticed that whether we set q or q' to unity is not relevant and we always arrive at

$$\frac{1}{T} = k \Xi_{gh}^{1-q} \frac{\mathfrak{S}'_1(E - mg\alpha, mg\bar{L})}{(\mathfrak{S}_1(E - mg\alpha, mg\bar{L}))^q}, \quad (5.31)$$

the temperature relation corresponding to the Tsallis q -entropy. Though the internal energy and the specific heat can be obtained from (5.31) in the $L \rightarrow \infty$ limit, there is no need to use the large N limit unlike the two parameter case.

VI Conclusions

In the current work we investigate the adiabatic class of ensembles in the framework of generalized statistical mechanics based on Schwämmle-Tsallis (q, q') entropy. We do not study the isothermal class of ensembles since the canonical treatment carried out in [23] can be extended to the other members of the class which includes the isothermal-isobaric, the grandcanonical and the generalized ensembles. We provide a unified description of the adiabatic class of ensembles which includes the microcanonical (N, V, E) , isoenthalpic-isobaric (N, P, H) , the (μ, V, L) ensemble, and the (μ, P, R) ensemble. A generalized form of the equipartition theorem, the virial theorem and the adiabatic theorem are obtained. We investigate the nonrelativistic classical ideal gas in all the four ensembles. In the microcanonical, and the isoenthalpic-isobaric ensemble the entropy could be found for an arbitrary number of particles. Using the large N -limit, the heat functions obtained in terms of the temperature are expressed through the Lambert's W -function. From the heat functions the respective specific heats are evaluated. To the best of our knowledge an exact evaluation of the phase space volume in the (μ, V, L) and the (μ, P, R) ensembles has not been done so far. We in our current work assume a large N limit and compute the approximate phase space volume. From the phase space volume the entropy, the heat function and the specific heat of the classical ideal gas is found. The heat function and the specific heat are obtained in terms of the Lambert's W -function without any further approximation. The preconditions that the entropy should be concave and the heat function should be a continuous function of the deformation parameter restricts our choice of the W -function to the principal branch. The two parameter entropy is concave only in the region where $q + q' > 1$ excluding the zone $0 < (q, q') < 1$ where the entropy is not always concave and we analyze the specific heats only in the above mentioned region. For the microcanonical and the isoenthalpic-isobaric ensemble the specific heat is positive in the region for which both q and q' are greater than one and in the region where $q' > 1$ and $-\infty < q < 1$. But it is negative in the region $q > 1$ and $-\infty < q' < 1$. In the regime where the entropy is concave, the heat capacities of the (μ, V, L) and the (μ, P, R) ensembles are +ve when $q > 1$ and -ve if $q < 1$. The microcanonical specific heat of classical ideal gas and a system of hard rod gas confined in a finite region of space and subjected to gravity is also analyzed. The entropy and the specific heat are initially calculated as a function of internal energy exactly. But when we assume the height to

be infinite and the number of particles to be very large, the internal energy could be obtained as a function of temperature in terms of the Lambert's W -function. Again only the principal branch of the W -function contributes to the internal energy and the specific heat. In the case of the hard rod gas, the free length \bar{L} and the factor $E - mg\alpha$ plays a role analogous to the height and the energy in the classical ideal gas.

The investigation of the adiabatic ensembles by using the large N limit developed in the current article may be extended to other entropies like the κ entropy [11] and the two parameter Sharma-Mittal-Taneja entropy [19,20]. This may help us in knowing the similarities and differences in the thermostistical structure of different entropies. Such an understanding may help us to choose the generalized entropy which may describe a given complex system in the best possible manner. Further, construction of a Laplace transform based on the two parameter exponential may be of great help in establishing the connection between the isothermal and the adiabatic class of ensembles. But this is beyond the scope of the current work and will be pursued in future.

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